Schrödinger operators and canonical systems via spectral theory (Research on structure of operators using operator means and related topics)

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数理解析研究所講究録 第2113巻 2019年 33-40

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by

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Abstract

In this survey article we explore Schrödinger operators and canonical systems via (inverse) spectral theory. After reviewing some basic materials, we summarize several well-known results on spectra of Schrödinger operators. Then (inverse) spectral theory for Schrödinger operators and canonical systems will be investigated.

1 Schrödinger operators and their spectra

Let us start with one-dimensional (half-line) Schrödinger operators

$$S = -\frac{d^2}{dx^2} + V(x) \tag{1}$$

on $L^2(0, \infty)$, where V are real-valued locally integrable functions, called potentials. The corresponding Schrödinger eigenvalue equations (SEEs, in short) are

$$-y''(x,z) + V(x)y(x,z) = zy(x,z), \quad x \in (0, \infty), \tag{2}$$

where $z \in \mathbb{C}$ is a spectral parameter. It is then well known [23, 25] that each operator (1) with boundary condition(s) at 0 and possibly at ∞ has a unique (essential) self-adjoint extension (or equivalently, Weyl-Titchmarsh m-function, which will be discussed later).

More precisely, put a boundary condition at 0,

$$y(0)\cos\alpha - y'(0)\sin\alpha = 0 \tag{3}$$

where $\alpha \in [0, \pi)$. When no more condition at ∞ is necessary to extend, (1) is called in a *limit point case* at ∞, and otherwise, in a *limit circle case* at ∞. It turns out that being in a limit point case is equivalent to the fact that there exists a solution to the associated SEE (2) which is not square-integrable near ∞. (Or S is essentially self-adjoint.) For a limit circle case, all solutions to (2) are in $L^2(0, \infty)$.

From now on we assume, for convenience, that S is in a limit point case at ∞ and set $\alpha = 0$ (so Dirichlet boundary condition at 0), unless we mention differently. In the viewpoint of (inverse) spectral theory, we are interested in all information about spectra for (1), denoted by $\sigma(S)$, such as location, type and weight. Since V is real-valued, S is (essentially) self-adjoint, which implies that its spectrum σ is in the real line. Based on Lebesgue decomposition (or the types of supports measured by Lebesgue measure), σ_c,

This work was supported by the Research Institute for Mathematical Sciences, a Joint Usage/Research Center located in Kyoto University.

σ_s, σ_{ac}, σ_{sc} and σ_p are continuous, singular, absolutely continuous, singular continuous and point spectra respectively. Depending on the dimension of range of projection on each subset, essential and discrete spectra are denoted by σ_{ess} and σ_d respectively.

Normally the spectra $\sigma(S)$ have been investigated by asymptotic behavior of V near ∞, and the followings are well-known results:

I. Unbounded potentials near ∞ (even in weak sense, i.e., $V(x_{k_j}) \to \infty$ for some subsequence $\{x_{k_j}\}$). In this case $\sigma(S)$ has point spectrum only. This happens because its resolvent $(z - S)^{-1}$ becomes compact.

II. Bounded potentials.

- Basic example is the free Schrödinger operator (with Dirichlet boundary condition at 0), i.e., $V \equiv 0$. Then it is well-known that $\sigma = [0, \infty)$ and $\sigma_s = \emptyset$.
- It is well-known that any periodic potential has so-called *band structure*, i.e., similar to tiling its spectrum is the union of closed intervals which may touch but cannot overlap. This spectrum is purely absolutely continuous (that is, $\sigma_s = \emptyset$), since (to deal with periodic potentials) a new boundary condition at L (when L is the period of V) similar to (3) is first introduced, and then observe that the spectrum continuously depends on the given boundary condition. (Floquet theory!)
- Almost periodic and limit periodic potentials. Generically, their spectra would be a Cantor set. Typical example for these is so-called almost Mathieu operator on $\ell^2(\mathbb{Z})$
$$S_\omega^{\lambda,\alpha} u(n) = u(n+1) + u(n-1) + 2\lambda\cos(2\pi(\omega + n\alpha))u(n),$$
where $\alpha, \omega \in \mathbb{T}$ and $\lambda > 0$. (Purely ac when $\lambda < 1$, almost surely sc when $\lambda = 1$ and almost surely pure point spectrum when $\lambda > 1$. Moreover, its spectrum is a Cantor set for all irrational α and $\lambda > 0$. Ten martini problem!)
All examples for almost periodic potentials had ac spectrum. So Kotani-Last conjecture guessed this. Avila, Yuditskii and Volberg, however, disproved this conjecture, i.e., they found some almost periodic potential which does not have ac spectrum.

III. Decaying potentials, i.e., $V(x) \to 0$ as $x \to \infty$.

- [Weyl] $\int_n^{n+1} |V(x)|dx \to 0 \Longrightarrow \sigma_{ess} = [0, \infty)$.
- [L^1-potential] If V is integrable near ∞, then $\sigma_s \cap (0, \infty) = \emptyset$.
- [L^2-potential, Deift & Killip] If V is square-integrable, $\sigma_{ac} = [0, \infty)$.
- [Neumann and Wiguer] $V(x) = O(\frac{1}{1+x}) \Longrightarrow \sigma_p \cap (0, \infty) \neq \emptyset$. Typical Neumann potential $V(x) = 2kg\frac{\sin 2kx}{x}$ has a point spectrum at k^2.
- [Naboko] If $|V(x)| \leq \frac{C(x)}{1+x}$ where $C(x) \to \infty$, then $\sigma_{pp} = \overline{\sigma}_p = [0, \infty)$.
- Sparse potentials have $(0, \infty)$ as purely singular continuous spectrum.

2 Weyl m-functions and Herglotz functions

Let's talk about so-called Weyl-Titchmarsh m-functions for Schrödinger operators (1). Similar to (3) put a boundary condition at 0,

$$y(0)\cos\alpha - y'(0)\sin\alpha = 0$$

where $\alpha \in [0, \pi)$. For $0 < b < \infty$, we place another boundary condition at b,

$$y(b)\cos\beta + y'(b)\sin\beta = 0 \tag{4}$$

with another real number β in $[0, \pi)$. Note that β is used as a parameter for (4). When $b = \infty$, So-called Weyl theory says that, if (1) is in a limit point case at ∞, no more boundary condition except (3) is needed. However, if (1) is in a limit circle case at ∞, that is, every solution of (2) is in $L^2(0, \infty)$, then it is necessary to have a limit type boundary condition at ∞ as follows: Put $f(x, z) := u_\alpha(x, z) + m(z)v_\alpha(x, z)$, where u_α and v_α are the solutions to (2) satisfying the initial conditions, $u_\alpha(0, z) = v'_\alpha(0, z) = \cos\alpha$ and $-u'_\alpha(0, z) = v_\alpha(0, z) = \sin\alpha$. Then $m(z)$ is on the limit circle if and only if

$$\lim_{N\to\infty} W_N(\bar{f}, f) = 0 \tag{5}$$

where W_N is the Wronskian at N, that is, $W_N(f, g) = f(N)g'(N) - f'(N)g(N)$ and $\bar{f}$ is the complex conjugate of f. Similar to the case when $0 < b < \infty$, β is made use of as a parameter for these boundary conditions at ∞. See [5, 24] for more details.

Then (1) with (3) and possibly either (4) or (5) has a unique m-function $m^S_{\alpha,\beta}$ and it can be expressed by

$$m^S_{0,\beta}(z) = \frac{\tilde{y}'(0, z)}{\tilde{y}(0, z)} \quad \text{or} \quad m^S_{\alpha,\beta}(z) = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \cdot m^S_{0,\beta}(z) \tag{6}$$

where $\tilde{y}$ is a solution to (2) which is square-integrable near ∞ when (1) is in a limit point case at $b = \infty$, or which is satisfying either (4) when $0 < b < \infty$ or (5) when (2) is in a limit circle case at $b = \infty$. Here $\cdot$ means the action of a $2{\times}2$ matrix as a linear fractional transformation (which will be reviewed soon). For convenience $m^S_{\alpha,\beta}$ are called Schrödinger m-functions. They are *Herglotz functions*, that is, they map the upper half plane $\mathbb{C}^+$ holomorphically to itself. See e.g. [14] for all these properties of $m^S_{\alpha,\beta}$.

Before going further, let us recall the action of linear fractional transformations, based on [20]. A *linear fractional transformation* is a map of the form

$$z \mapsto \frac{az + b}{cz + d}$$

with $a, b, c, d \in \mathbb{C}$, $ad - bc \neq 1$. This can be expressed very easily via matrix notation by

$$A \cdot z = \frac{az + b}{cz + d}, \quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

This notation has a natural interpretation: Identify $z \in \mathbb{C} \subset \mathbb{CP}^1$ with its homogeneous coordinates $z = [z : 1]$ and apply the matrix A to the vector $\left(\begin{smallmatrix} z \\ 1 \end{smallmatrix}\right)$ whose components are these homogeneous coordinates. The image vector $A\left(\begin{smallmatrix} z \\ 1 \end{smallmatrix}\right)$ then reveals what the homogeneous coordinates of the image of z under the linear fractional transformation are.

Even though Schrödinger m-functions are Herglotz functions, the converse is not true. To verify this let us see that, because of the Herglotz representation, not all Herglotz functions can have the asymptotic behavior which Schrödinger m-functions should do. Indeed, Everitt [6] showed that, when $z \in \mathbb{C}^+$ is large enough, $m^S_{\alpha,\beta}$ satisfy the asymptotic behavior

$$m^S_{0,\beta}(z) = i\sqrt{z} + o(1) \tag{7}$$

for $\alpha = 0$, or

$$m^S_{\alpha,\beta}(z) = \frac{\cos\alpha}{\sin\alpha} + \frac{1}{\sin^2\alpha}\frac{i}{\sqrt{z}} + O\big(|z|^{-1}\big) \tag{8}$$

for $\alpha \in (0,\pi)$. See also [1, 9] for more developed versions of the asymptotic behavior of $m^S_{\alpha,\beta}$. Given a Herglotz function F, it can be expressed by

$$F(z) = A + \int_{\mathbb{R}_\infty} \frac{1+tz}{t-z} d\rho(t) \tag{9}$$

where A is a real number and $d\rho$ is a finite positive Borel measure on $\mathbb{R}_\infty$, the one-point compactification of the set of all real numbers $\mathbb{R}$. (See e.g. (2.1) in [19].) Then (9) indicates that any Herglotz function with a measure $d\rho$ having a positive point mass at ∞ cannot satisfy (7) nor (8), and therefore it is not a Schrödinger m-function. However, for $d\rho$ to be a measure associated with (1) (or so called spectral measure), a more issue is on the asymptotic behavior of $d\rho$ near ∞. See two sections 17 and 19 of [18] for details.

Now let us see why these m-functions are useful in order to investigate the spectra of Schrödinger operators. First, it turns out that in Borg and Marchenko [2, 15] this Weyl m-function uniquely determines the potential V and the boundary condition at 0. Moreover, this m-function characterizes its spectrum of S as follows: let $\Omega = \{t \in \mathbb{R} : \lim_{\epsilon\downarrow 0} \operatorname{Im} m^S_{\alpha,\beta}(x+i\epsilon) \text{ exists}\}$ (recall that $|\mathbb{R}\setminus\Omega| = 0$, i.e., Ω is Lebesgue measure zero).

- $\Sigma = \{t \in \Omega : 0 < \operatorname{Im} m^S_{\alpha,\beta}(x) \le \infty\}$
- $\Sigma_{ac} = \{t \in \Omega : 0 < \operatorname{Im} m^S_{\alpha,\beta}(x) < \infty\}$
- $\Sigma_s = \{t \in \Omega : \operatorname{Im} m^S_{\alpha,\beta}(x) = \infty\}$
- $d\rho(x) = \lim_{\epsilon\downarrow 0} \frac{1}{\pi}\operatorname{Im} m^S_{\alpha,\beta}(x+i\epsilon)dt$ in weak-$*$ sense
- $\rho(\{x\}) = \lim_{\epsilon\downarrow 0} \epsilon \operatorname{Im} m^S_{\alpha,\beta}(x+i\epsilon)$

where $\Sigma_{(\cdot)}$ presents almost the support of the related spectral measure ρ by Lebesgue decomposition (i.e., absolute and singular parts of this measure) and this m recovers ρ in weak sense. All this means that these m-functions have the full information for the spectra of (1).

3 Canonical systems and de Branges theory

In the previous subsection we saw that not every Herglotz function is an m-function of a Schrödinger operator. To see a general connection between Herglotz functions and differential equations let us consider more generally a half-line canonical system,

$$Ju'(x,z) = zH(x)u(x,z), \quad x \in (0,\infty) \tag{10}$$

where H is a positive semidefinite 2×2 matrix whose entries are real-valued, locally integrable functions and $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$. A canonical system (10) is called *trace-normed* if $\operatorname{Tr} H(x) = 1$ for almost all x in $(0, \infty)$. For (10) we always place a boundary condition at 0,

$$u_1(0, z) = 0 \tag{11}$$

where u_1 is the first component of $u = \left(\begin{smallmatrix} u_1 \\ u_2 \end{smallmatrix}\right)$. Similar to (6), its m-function, m_H, can be expressed by

$$m_H(z) = \frac{\tilde{u}_2(0)}{\tilde{u}_1(0)}$$

where $\tilde{u} = \left(\begin{smallmatrix} \tilde{u}_1 \\ \tilde{u}_2 \end{smallmatrix}\right)$ is a solution to (10) satisfying

$$\int_0^\infty \tilde{u}^*(x) H(x) \tilde{u}(x) dx < \infty. \tag{12}$$

Here * means the Hermitian adjoint. Such a solution satisfying (12) is called *H-integrable.* See [26, 27] for all these properties of (10).

One of the difficulties with canonical systems is that we may not define an operator related to this system. Especially, when H is not invertible, we cannot obtain an operator, but a relation. However, it is well-known that we are able to apply (self-adjoint) spectral theory on the relation from (10) . See [10] for more details.

Recall that there were three cases when defining Schrödinger m-functions and in each case we needed a special solution to formulate the corresponding m-function. For (10) an H-integrable solution, however, is only needed, since (10) is half-line and a half-line trace-normed canonical system is always in a limit point case at ∞. In other words, there is only one H-integrable solution up to a multiplicative constant. See the original argument by [3] for more details.

More importantly De Branges [4] and Winkler [26] showed the one-to-one correspondence between Herglotz functions and canonical systems, i.e., for a given Herglotz function, there exists a unique half-line trace-normed canonical system with (11), such that its m-function m_H is the given Herglotz function. This one-to-one correspondence is essential in order to cope with canonical systems rather than Herglotz functions or their m-functions.

4 Inverse spectral theory for Schrödinger operators and canonical systems

In spectral theory of operators, we would like to inspect the spectra of given operators. Reversely, for a given subset of the real line or more generally a given spectral measure (which looks like ρ in the previous section), we would want to characterize the operators which have the given set as their spectra. Now let's summarize these inverse spectral theories on Schrödinger operators and canonical systems.

- Not all Herglotz functions are Schrödinger m-functions, which we saw due to the asymptotic behavior near ∞.
- There is 1-1 correspondence between (trace-normed) canonical systems and Herglotz functions.

- There are several complete descriptions for Schrödinger m-functions (see [7, 8, 13, 16, 17, 18, 21] for more details), but they are difficult to apply.
- There is 1-1 correspondence between Jacobi operators (which are considered as generalization of discrete version of Schrödinger operators) in [22] and spectral measures having infinite but compact support.
- For the discrete Schrödinger operators, there is no general inverse spectral theory.

Based on these facts, we may ask ourselves why we have difficult inverse spectral theory of Schrödinger operators rather than discrete ones. To see this reason we would like to present two recent results in [11, 12].

Theorem 4.1 (Theorem 3.1 in [11]) *The space of Schrödinger m-functions with some fixed boundary condition α at 0 is dense in the space of all Herglotz functions.*

This theorem is actually stronger than it is, in the sense that the potentials V can be chosen from smooth functions. Also this asserts that we have enough Schrödinger m-functions or Schrödinger operators compared to all Herglotz functions or canonical systems, respectively. Unlike this continuous setting, for discrete one we do not have the density.

Theorem 4.2 (Theorem 4.2 in [12]) *There is a Jacobi operator whose m-function cannot be approximated by the m-functions for discrete Schrödinger operators in the sense of the local uniform convergence.*

Even though we have very nice inverse spectral theory for Jacobi operators, due to the rarity of discrete Schrödinger operators compared to Jacobi ones, it is extremely difficult to have a general inverse spectral theory for discrete ones.

To show these two theorems we characterize the canonical systems corresponding to Schrödinger operators and discrete Schrödinger operators respectively (which are Proposition 4.1 in [11] and Theorem 3.2 in [12] respectively). Most importantly these characterizations are very easy to apply. Indeed, by looking at several conditions we can easily check if the given canonical systems are related to (discrete) Schrödinger operators. With the convergence from de Branges on canonical systems we are able to show the density or no-density of the continuous or discrete Schrödinger operators. Please see [11, 12] for all details.

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